Pacific Northwest National Laboratory's Hydrogen Analysis Capabilities

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DOE Hydrogen, Fuel Cells, and Infrastructure Technologies Program

Systems Analysis Workshop

July 28-29, 2004

Washington, D.C.

Battelle

Charter

- **PNNL Energy Science and Technology Directorate's Energy Mission*:***
  Secure, clean, and affordable energy systems in a carbon constrained world.

- **PNNL Analysis Objectives/Principles**:
  - Development of **state-of-the-art** analysis tools for critical policy issues (e.g., climate change, electricity grid issues)
  - Use of tools **appropriate** to the need
  - **Objectivity**; analysis based on best available, un-biased data and assumptions

- **Analysis Funding Sources:**
  - DOE/EERE (including HFCIT, FreedomCar, Biomass, IT, BT, DEER, PBA)
  - DOE/SC (integrated assessment modeling)
  - DOE/NA (nuclear hydrogen production study)
  - DOE/OETD (GridWise modeling)
  - DoD – e.g., Army, DARPA
  - Private Sector (integrated assessment modeling, and special studies for private companies)
  - LDRD (PNNL has initiatives in hydrogen, carbon management, and energy systems transformation [GridWise])

History

- Long history of analysis work at PNNL: ~25+ yrs
- Past analysis projects in cost analysis, lifecycle analysis, market analysis, decision analysis, systems optimization, systems comparision for a variety of technologies (see backup slides)
- Hydrogen has been included in PNNL integrated assessment models for 10 years or so

PNNL Tools

Across the Scale and Scope Spectrum

Scale: Components → Technology Systems → Global Energy, Economic, Environmental System

Scope:

Energy/Materials

Environment

Economics

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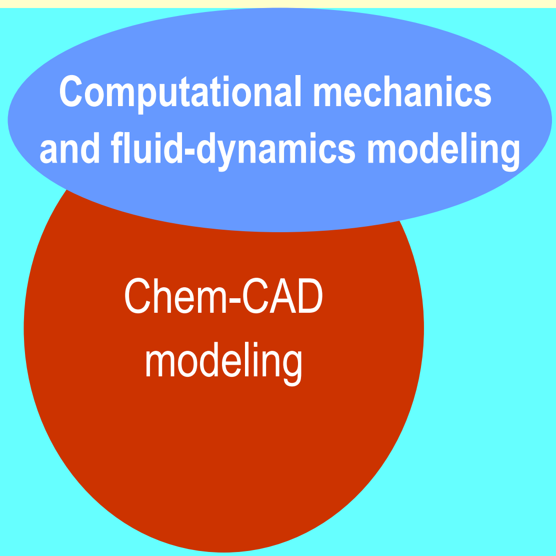

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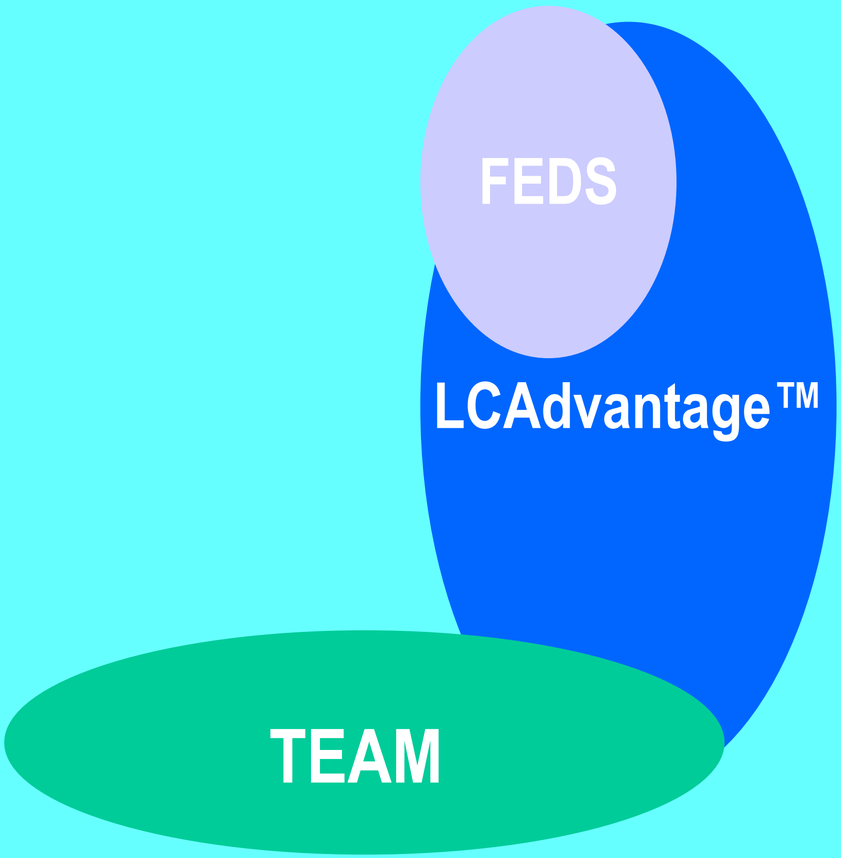

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Across the Scale and Scope Spectrum

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GRIDLAB-D and -T

Integrated Assessment Models:
SGM
MiniCAM
ObjECTS

PNNL Tools

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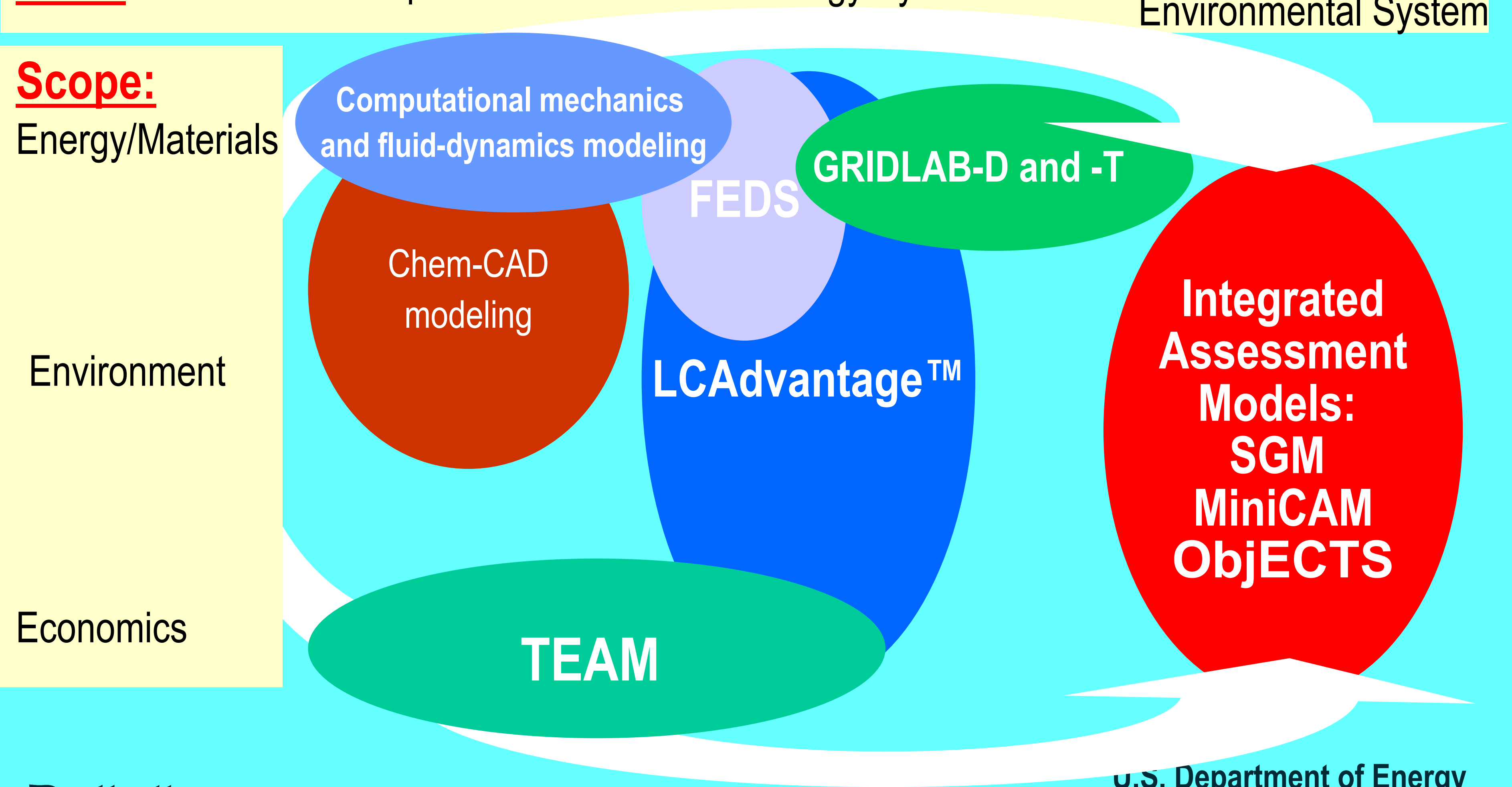


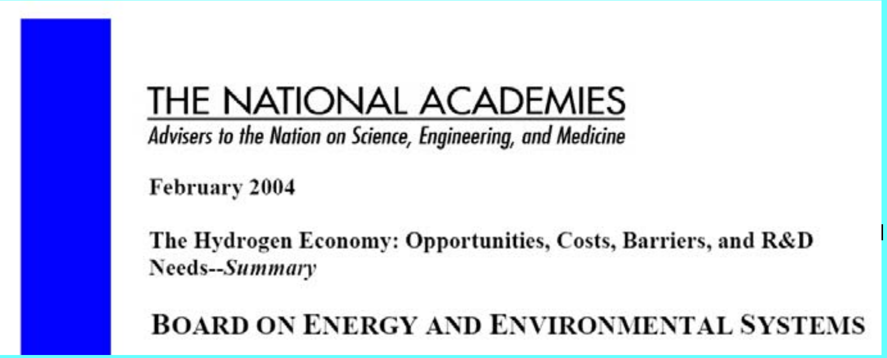
Skill Set - People

People	Group or Initiative	Capabilities
George Muntean et al.	Computational Mechanics and Material Behavior Group	Materials components modeling using ANSYS, ABACUS and other commercial codes (H_2 Storage)
Don Stevens, Todd Werpy, et al.	Chemical and Biological Process Group	Chemical process modeling, e.g., biomass systems (mostly using Chem-CAD)
Daryl Brown, Jim Dirks, Mark Weimar et al.	Technology Systems Analysis Group; TPD Group	Technology assessment; lifecycle costing; TEAM, FEDS
Marylynn Placet et al.	Energy Policy and Planning Group (DC)	Financial analysis, strategic planning, program benefits assessment
Rob Pratt, Landis Kaanberg, et al.	Energy Technology Development Group; GridWise Initiative	Modeling/simulation of electricity markets and infrastructure: GRIDLAB-D and –T
Jae Edmonds et al. Charlette Geffen Ken Humphreys	Joint Global Change Research Center (DC); Carbon Management Initiative	Integrated assessment modeling: SGM, MiniCAM, ObjECTS

Skill Set – Models that Currently Include Hydrogen (1)

- **SGM - MiniCAM - ObjECTS**
  - SGM, MiniCAM and ObjECTS currently in use; ObjECTS is a new framework developed in 2004
  - Global/partial equilibrium model of the economy, with emphasis on the energy sector. Makes 50 to100-year projections of energy patterns, emissions, costs
  - Part of integrated assessment modeling system targeted toward understanding global climate issues
  - Versions under development are using object-oriented modeling approach (C^{++}); we do not use a commercial modeling platform
  - *Limitations*: Hydrogen infrastructure costs included but infrastructure constraints not modeled. Currently expanding detail on end-use building services to better address hydrogen technologies in buildings.

From the NAE Study to ObjECTS.MiniCAM


THE NATIONAL ACADEMIES

Advisers to the Nation on Science, Engineering, and Medicine

February 2004

The Hydrogen Economy: Opportunities, Costs, Barriers, and R&D Needs--*Summary*

BOARD ON ENERGY AND ENVIRONMENTAL SYSTEMS

- Introduced the NAE technological assumptions into the new **ObjECTS/MiniCAM** modeling system.
  - Long-term, global integrated assessment model of energy, economy and climate change
  - 14 global regions,
  - Time horizon of 2095
- Took the NAE engineering data as assumptions
- Used the ObjECTS/MiniCAM to analyze market competition and energy-economy interactions.
  - H_2 in transportation, stationary applications, interactions with other energy supply and transformation technologies.

Going Beyond the NAE Study

Four Cases Selected to Frame an Initial Assessment

Two Technology States of the World

- Reference technology (Ref 2100)
- Advanced (NAE) technology (Adv 2100)

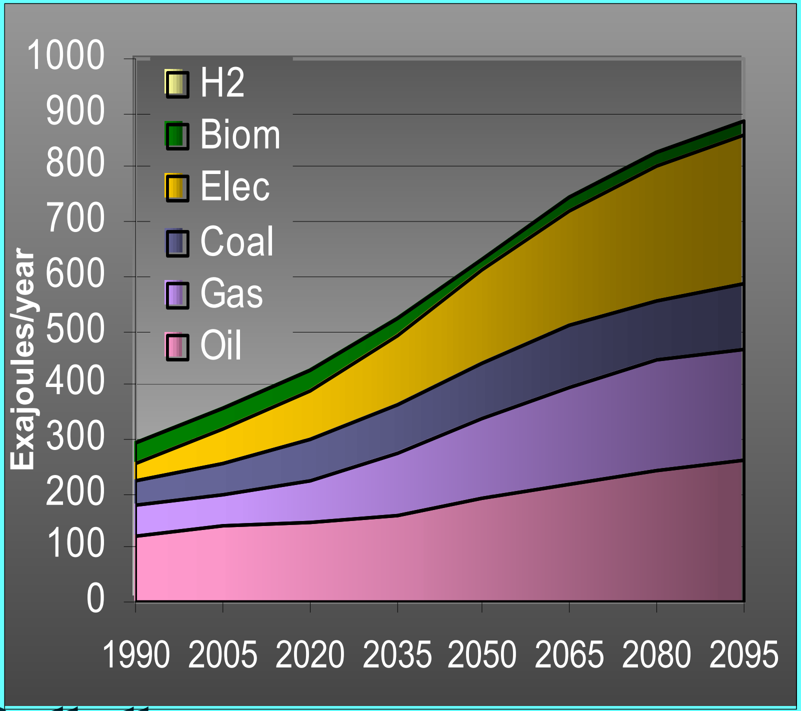
Two Policy States of the World

- No explicit climate policy imposed (no constraints)
- Climate policy where concentrations are constrained to 550 parts per million volume (ppmv)

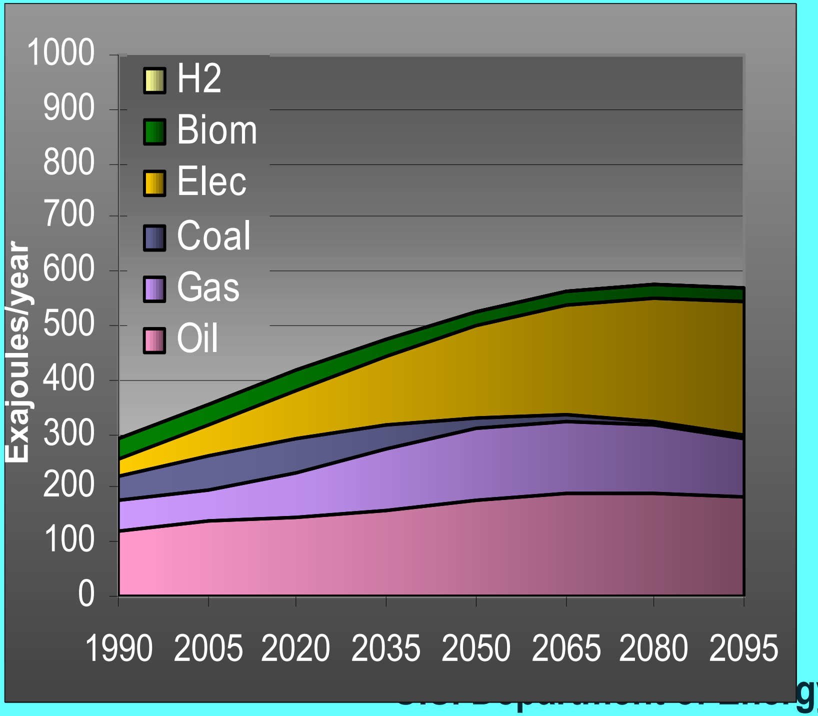
Initial Findings

Climate change policy alone does not necessarily create a market for hydrogen—the technology has to be market competitive without climate policy.

Reference Case, End-use Energy



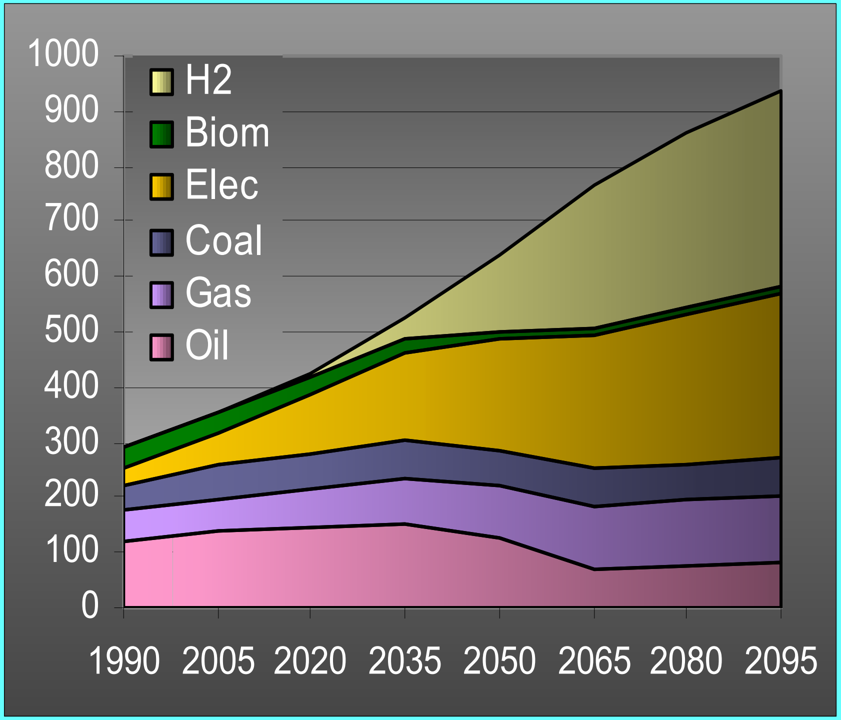
Reference Case Technology, End-use Energy—550 ppm CO_2



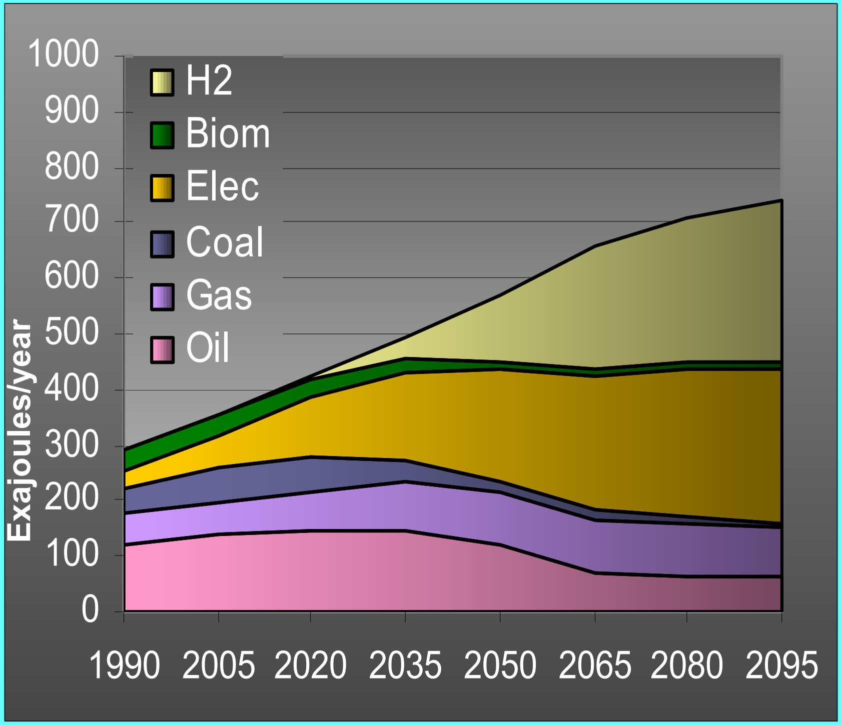
Initial Findings

The introduction of a carbon constraint may actually reduce the deployment of hydrogen, although H_2 maintains relative market share

H_2 and CCS Technology Case, End-use Energy—No Climate Policy



H_2 & CCS Technology Case End-use Energy—550 ppm CO_2



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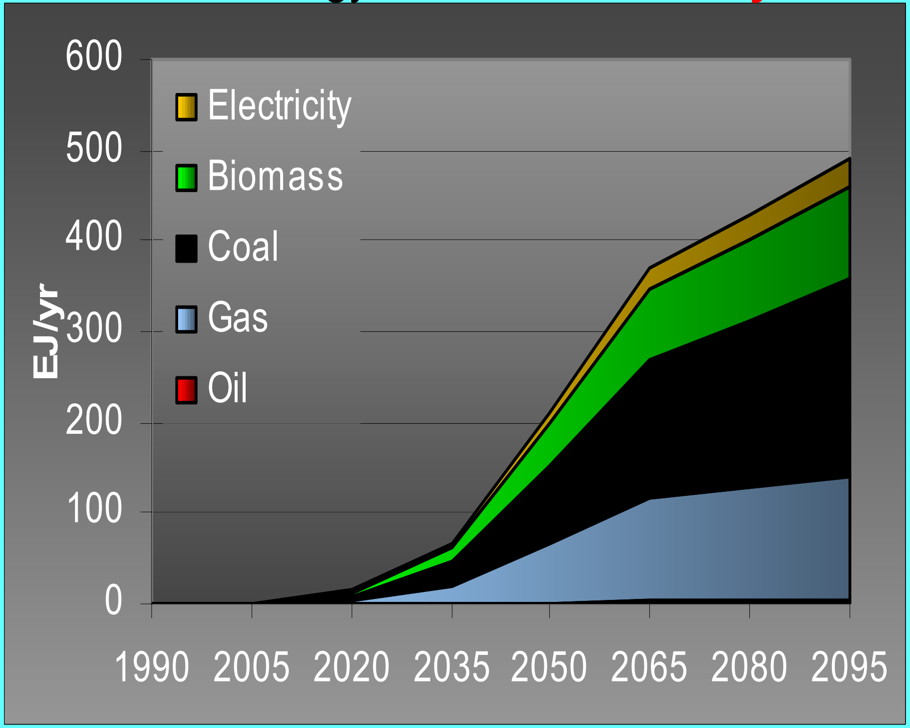
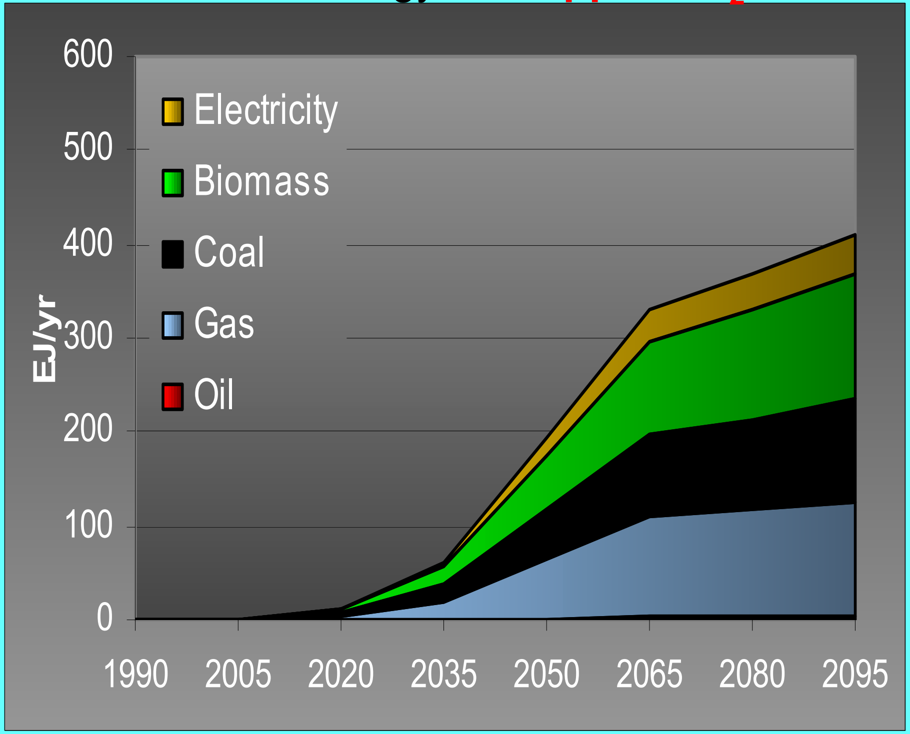
Initial Findings

Hydrocarbons may be the most attractive hydrogen feedstocks. The composition shifts toward bio-fuels in a climate-constrained world.

H_2 and CCS Technology Case, End-use Energy—**No Climate Policy**



H_2 & CCS Technology Case End-use Energy—**550 ppm CO_2**



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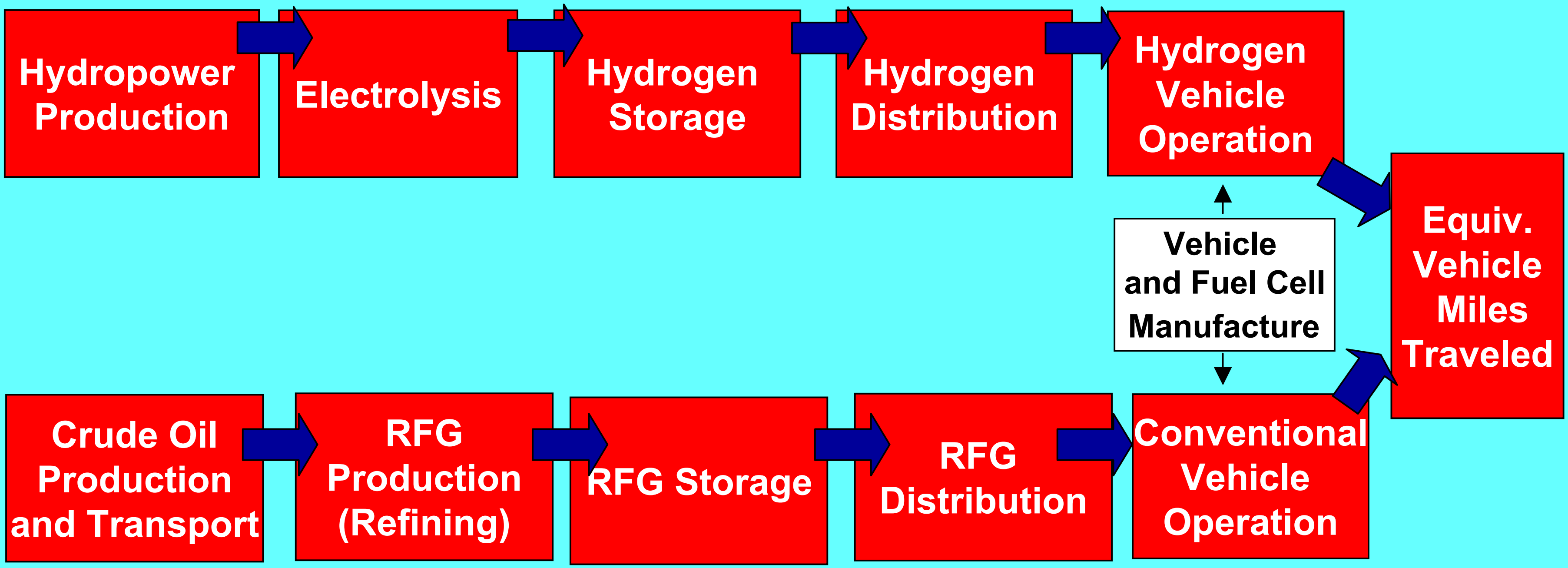
Skill Set – Models that Currently Include Hydrogen (2)

- **LCAdvantage™**
  - Developed in mid-1990s; won R&D100 award
  - Life-cycle inventory tool with economic accounting capability. Characterizes the energy, economic, and environmental impacts of products and processes over their full cradle-to-grave life cycles.
  - Self-contained, written in C++, runs on any Windows computer
  - Modest LDRD effort directed toward introducing hydrogen technologies
  - *Limitations:* Model produces a snapshot in time for a system, and is not a dynamic simulation.

Potential Application of LCAdvantage™ to Hydro-Produced Hydrogen

Stages in the Hydrogen-Powered and Conventional Vehicle Energy Cycles



Characterize energy flows, lifecycle costs and environmental impacts for:

- each individual technology in the pathway
- the full energy cycle

Skill Set – Models that Could Potentially be Adapted to Include Hydrogen (1)

- **TEAM – "The" Economic Analysis Model**

Could be used to conduct lifecycle cost analysis of a wide range of hydrogen components, technologies, systems

- Flexible, EXCEL-based lifecycle cost analysis tool that generates year-by-year cash flow streams; calculates paybacks, discounted paybacks, IRR, profitability ratios, levelized costs
- Originally developed in 1987 in support of DOE Thermal Energy Storage Program, but developed in a technology-neutral format.
- Considers initial capital, interim capital, O&M, revenue, operating life, property tax rate, income tax rate, discount rate, inflation rate
- *Limitations*: Not completely "user friendly"

Skill Set – Models that Could Potentially be Adapted to Include Hydrogen (2)

- **FEDS – Federal Energy Decision System**

  Could be used to examine the economics of hydrogen use in building applications

  - Model development and use began in 1990 and continues to date.
  - Fuel-neutral, technology independent, comprehensive method for quickly and objectively identifying building energy technology improvements that offer maximum life-cycle cost savings
  - Hourly building simulation using typical day, hot day, and cold day for each month and day type (weekday, Saturday, and Sunday). FEDS uses a sequential iterative optimization approach to determine the minimum life-cycle cost for building technologies.
  - Model developed in C and C++ with a Visual Basic user interface and Access databases
  - *Limitations*: Has not been applied to fuels cells or other hydrogen-using technologies

Skill Set – Models that Could Potentially be Adapted to Include Hydrogen (3)

- **GRIDLAB-D (operational) and GRIDLAB-T (under development)**

Could be adapted to simulation of hydrogen distribution/delivery systems

- Tool for simulating the combined system performance and operation of the power grid's: (1) electric infrastructure; (2) electric loads at the end-use level including consumer behavior (3) new distributed resource technologies such as distributed generation, storage, and peak load demand response technologies for consumers, (4) wholesale and retail markets, contracts, and trading, including agent-based decision making on the part of buyers, sellers, and consumers
- GridWise-D: scope ranges from the distribution substation and retail markets to individual appliances cycling on and off in populations of ten's of thousands of individual buildings.
- GridWise-T: scope ranges from the substation load (feeder level) up to the transmission system and power plants, including operation of wholesale markets.
- Uses thermodynamic and behavioral/statistical models of end-use loads; partial differential power flow equations and grid control operations; agent-based models of human actors in markets and consumers. Coded in C++ (windows and linux) with MatLab Power Systems Toolkit (GridLab-D); Areva T&D Dispatch Training Simulator (GridLab-T)
- *Limitations:* Presently a research tool -- primitive user interface. It is still under development for public domain use. The simulation includes fuel-based end-uses but not fuel infrastructure or markets (yet).

Skill Set – Models that Could Potentially be Adapted to Include Hydrogen (4)

- **Process Engineering Tools**

  Could be applied by PNNL for engineering simulation and techno-economic analysis in PNNL technical specialty areas such as:

  - H_2 storage materials/systems
  - Microtechnology components in hydrogen systems
  - Bio-processes
  - Solid-oxide fuel cells

Skill Set – Capabilities Summary

TYPE OF ANALYSIS	RESIDENT CAPABILITY?	STUDIES SPECIFIC TO H_2?	MODELS SPECIFIC TO H_2?
Resource Analysis	Yes	Yes	Yes
Technoeconomic Analysis	Yes	Yes	Yes
Environmental Analysis	Yes	Yes, esp. for carbon emissions	Yes
Delivery Analysis	Yes, for electricity	No	No
Infrastructure Development Analysis	Yes	No	No
Energy Market Analysis	Yes	Yes	Yes

Hydrogen-Specific Studies

- Weimar et al. 2004. "Using a High-Temperature Hydrogen Co-Generation Reactor to Optimize both Economic and Environmental Performance" (Study conducted for DOE/NA; paper presented at NHA)

- Several JGCRI hydrogen papers, e.g.:
  - Edmonds. 2004. "Hydrogen Technologies: Setting the Policy Research Agenda." George Washington University, Hydrogen Systems in the Context of Addressing Climate Change.
  - Geffen, Edmonds, and Kim. 2004. "Transportation and Climate Change: The Potential for Hydrogen Systems." Presented at SAE 2004 World Congress.
  - Geffen, Edmonds and Kim. 2004. "Hydrogen and Climate Change: An Integrated Assessment of Long-Term Impacts." National Hydrogen Association meeting.

Future

Plans for the further development of PNNL's integrated assessment models include in-depth study of hydrogen technology/infrastructure for improvement of the model's treatment of hydrogen production, delivery and end use.

Analysis Issues

- What are the best end uses for hydrogen (is it mainly a solution for transportation, or does it make sense for distributed generation, buildings, etc.)? When and where does the hydrogen market develop?
- How much will delivered hydrogen cost? Can it compete with future alternatives? How will regional differences affect the cost?
- What sources will supply the hydrogen, and how does hydrogen production impact existing energy markets?
- What production and delivery scenarios make sense in each US region? When and where does central production make sense? What is the role for forecourt production (is it just a transition approach or does it make sense in the long-run)?

Analysis Issues (cont'd)

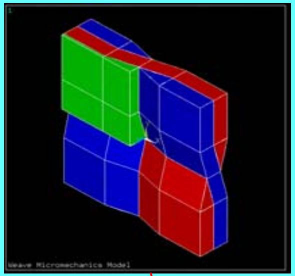
- What is the role of storage? Can production and storage be optimized to reduce overall costs, given a range of available production and storage technologies?
- How much will it cost to develop a hydrogen economy? What are the financing options?
- How will hydrogen markets develop outside the United States? How will such developments impact the hydrogen transition, prices, and technologies used in the US?
- To what extent does the availability of hydrogen lower carbon emissions from the transportation (and other) sectors? How would a carbon tax or other carbon policies impact hydrogen markets and hydrogen technology choice?
- What other kinds of policies might encourage hydrogen?

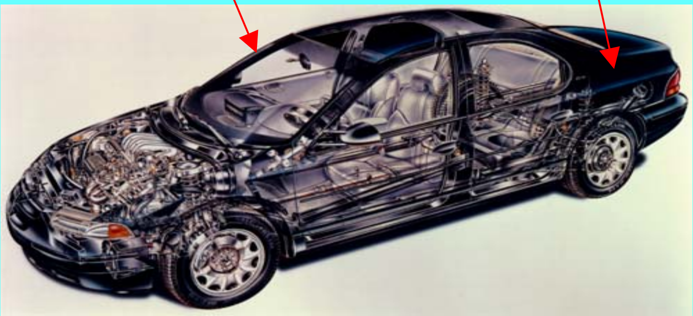
Backup Slides

Component Modeling

Computational Mechanics and Material Behavior Group

- Development of state-of-the-art simulation and modeling solutions to the industrial challenges in manufacturing lightweight vehicles and structures, vehicular air pollutant formation and controls, and **energy and fuel storage devices.**
- Work has focused primarily on materials that are critical to the development of lightweight, fuel-efficient cars and trucks:
  - Aluminum, Magnesium, Titanium
  - Glass
  - Thermoplastic composites
- Actively supporting research in:
  - new methods for joining dissimilar materials
  - hydroforming, superplastic forming, electromagnetic forming
- Baseline capabilities include
  - High performance computing
  - Collaborative tools
  - Engineering, materials/chemical sciences
- Applications
  - Manufacturing and materials
  - Emission control
  - Fuel cells & fuel storage





System Modeling Of Hydride Hydrogen Storage Cells

- Simulating this system will require a coupled field Structural/Thermal/Fluid-Dynamics analysis
  - May be doable entirely in ANSYS Multiphysics or may need to be split between ANSYS and StarCD as it is currently done in fuel cell analyses
- H_2 and hydride interaction is a key element of the analysis, and could be handled in a Fortran or C++ model
- System modeling could provide a great advantage when evaluating the suitability of new hydrides other storage methods by estimating:
  - Containment structure (size, materials, mass)
  - Energy requirements (external heating and cooling to drive the reactions)
  - System efficiency

Chemical and Biological Process Group

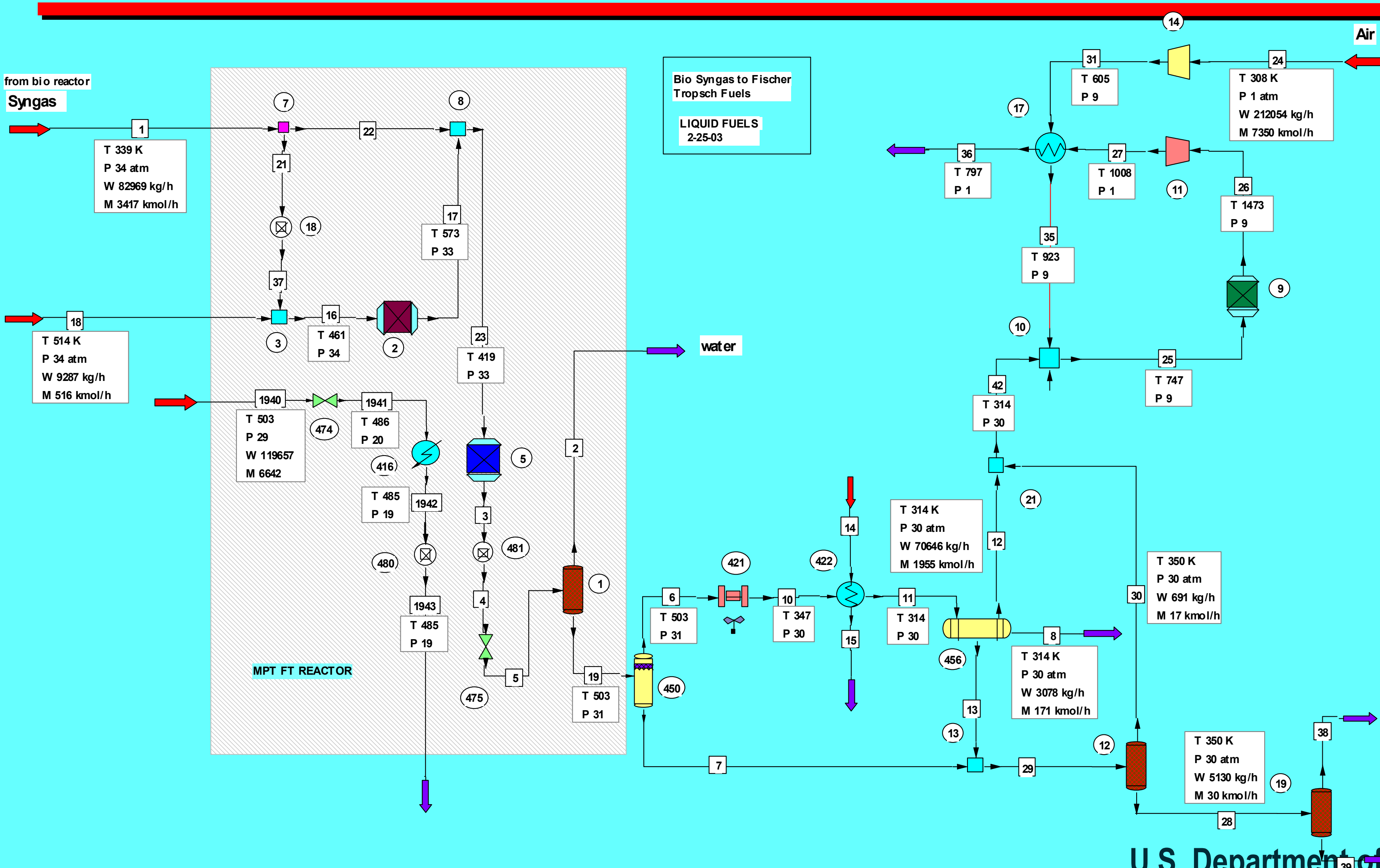
Chemcad flowsheets used as basis for equipment sizing and costing and/or for flow estimation

Recent activities:

- Prepared relative cost comparison between conventional technology and novel microtechnology reactor to produce Fischer-Tropsch fuels from biomass derived syngas (2003)
- Prepared Excel based spreadsheet cost models for use in evaluating biomass processing steps (glucose to products): aerobic and anaerobic fermentation, oxidation, hydrogenation, crystallization (2003)
- Updating Techno-Economic Analysis for pyrolysis oil upgrading via hydrotreating (2004)

Example of Recent Chemcad Analysis:

Microtech reactors to upgrade biomass-derived syngas to Fischer-Tropsch fuels



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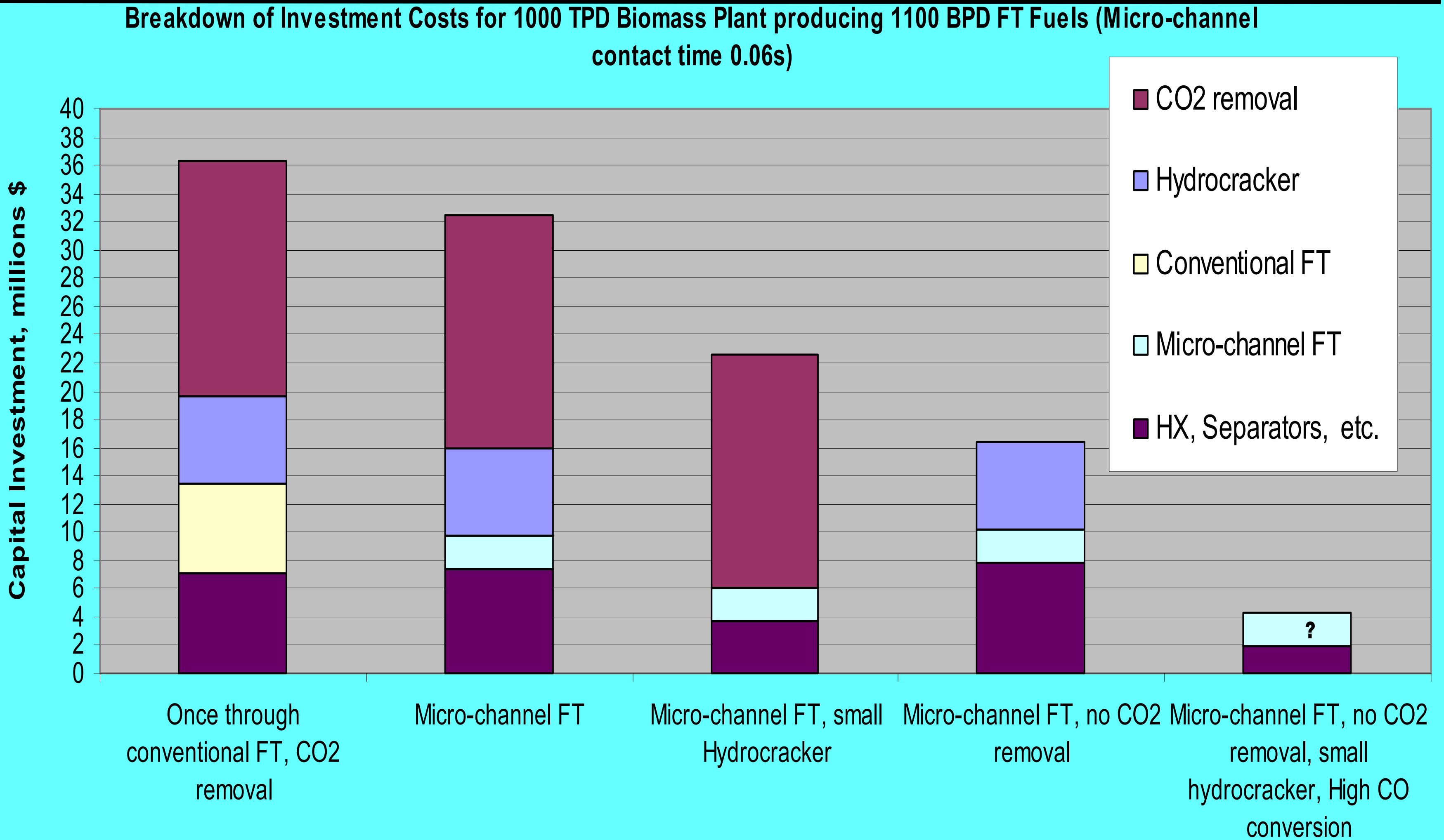
Cost comparisons



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Technology Systems Modeling

Facility Energy Decision System (FEDS)

An easy to use, yet powerful & flexible tool for quickly and objectively identifying building energy technology improvements

- Accepts generic or very detailed inputs and provides intelligent inferences for missing data
- Evaluates the cost and performance of thousands of building energy retrofit technologies, estimating energy consumption and electric demand (peak & coincident) for all energy systems
- Determines the minimum life-cycle-cost retrofits to systems within a facility and on an installation, considering all interactive effects

- Building Shell
- Advanced HVAC Options
  - Ground-coupled heat pumps
  - Dual-fuel heat pumps
  - Gas engine chillers
  - Absorption chillers
- Advanced Lighting Technologies
- Motors
- Refrigeration Equipment
- Plug Loads
- Central Energy Plants (coming soon)

Rebuild America

FEMP

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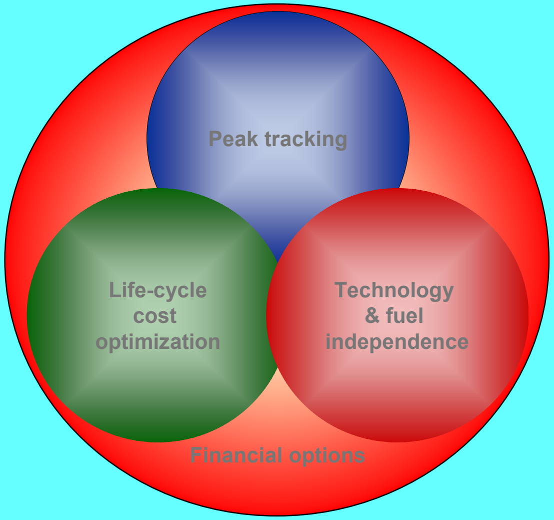
Facility Energy Decision System (FEDS)



- Examines single buildings to large multi-building installations
- Tracks emissions impacts
- Conducts alternative financing analyses
- Allows users to modify cost data & optimization parameters
- Models 16 civilian & 28 military building types
- Provides detailed output

www.pnl.gov/FEDS

Rebuild America

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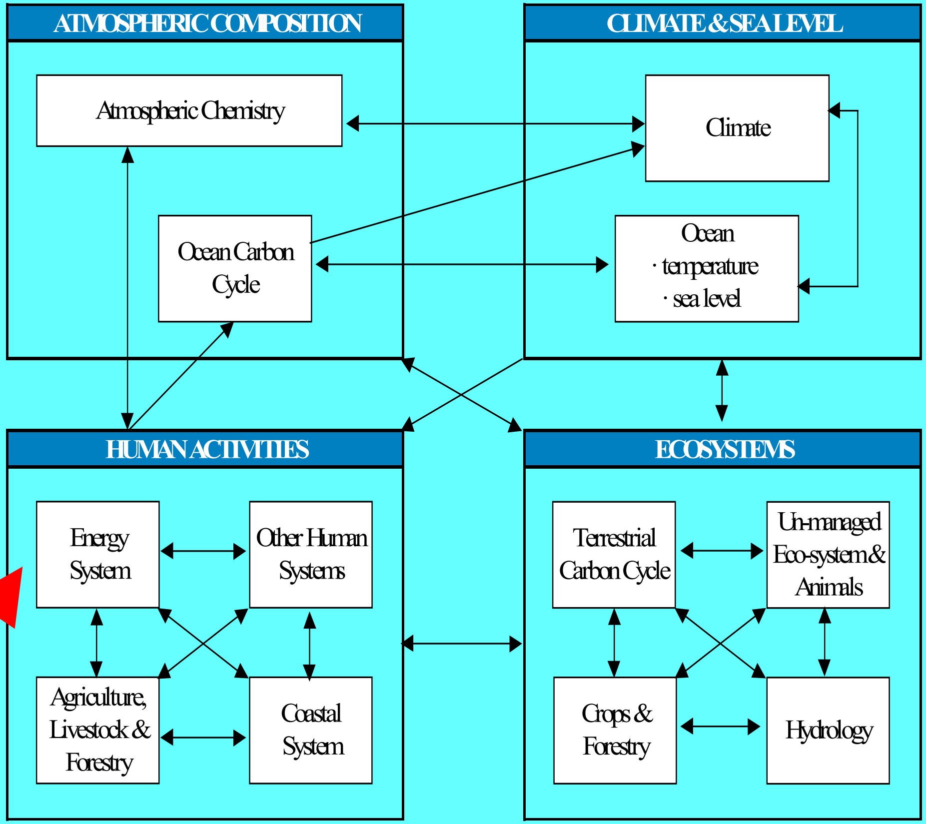
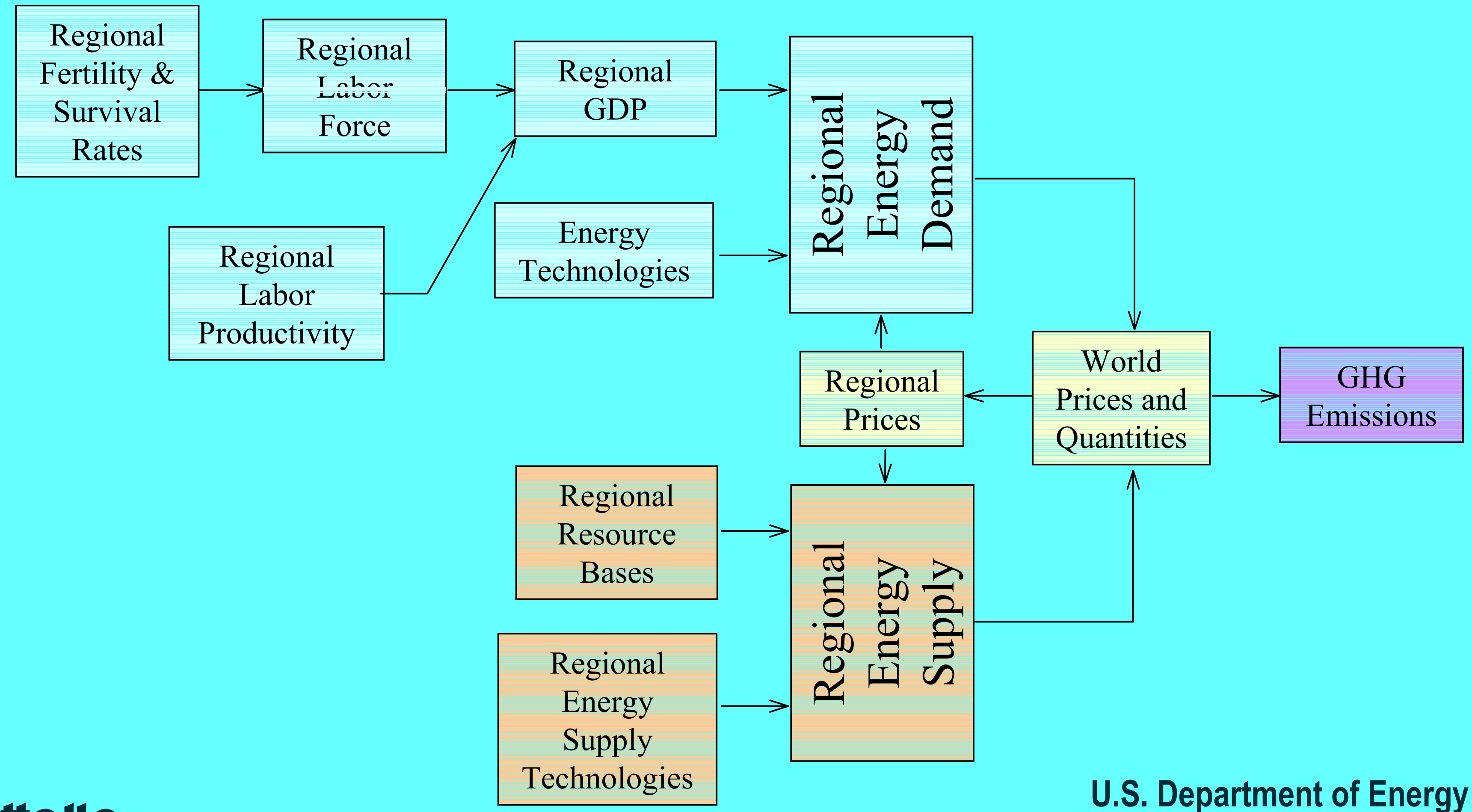
Integrated Assessment Modeling

An integrated assessment approach enables evaluation of the dynamics of technology evolution and change

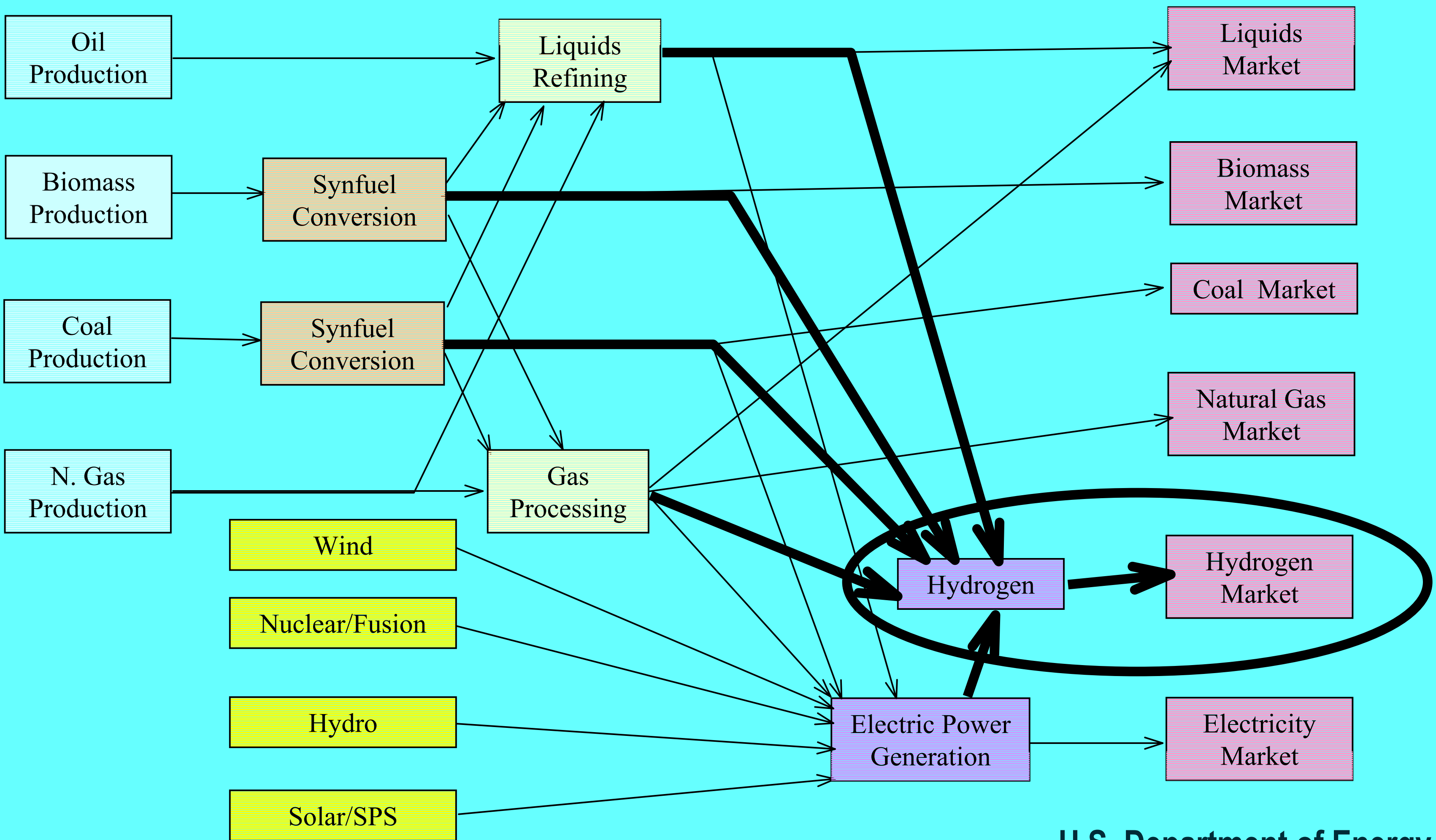
- Economics-based analysis of price and market share of new technologies under various future scenarios, and their greenhouse gas emissions
- Understand timelines and potential pathways for evolution of hydrogen energy systems
- Global framework for analysis, accounting for regional differences
- Context for evaluating the magnitude of infrastructure investment required by region



Core Elements of MiniCAM Energy Markets



Alternative production pathways for hydrogen represented in the MiniCAM



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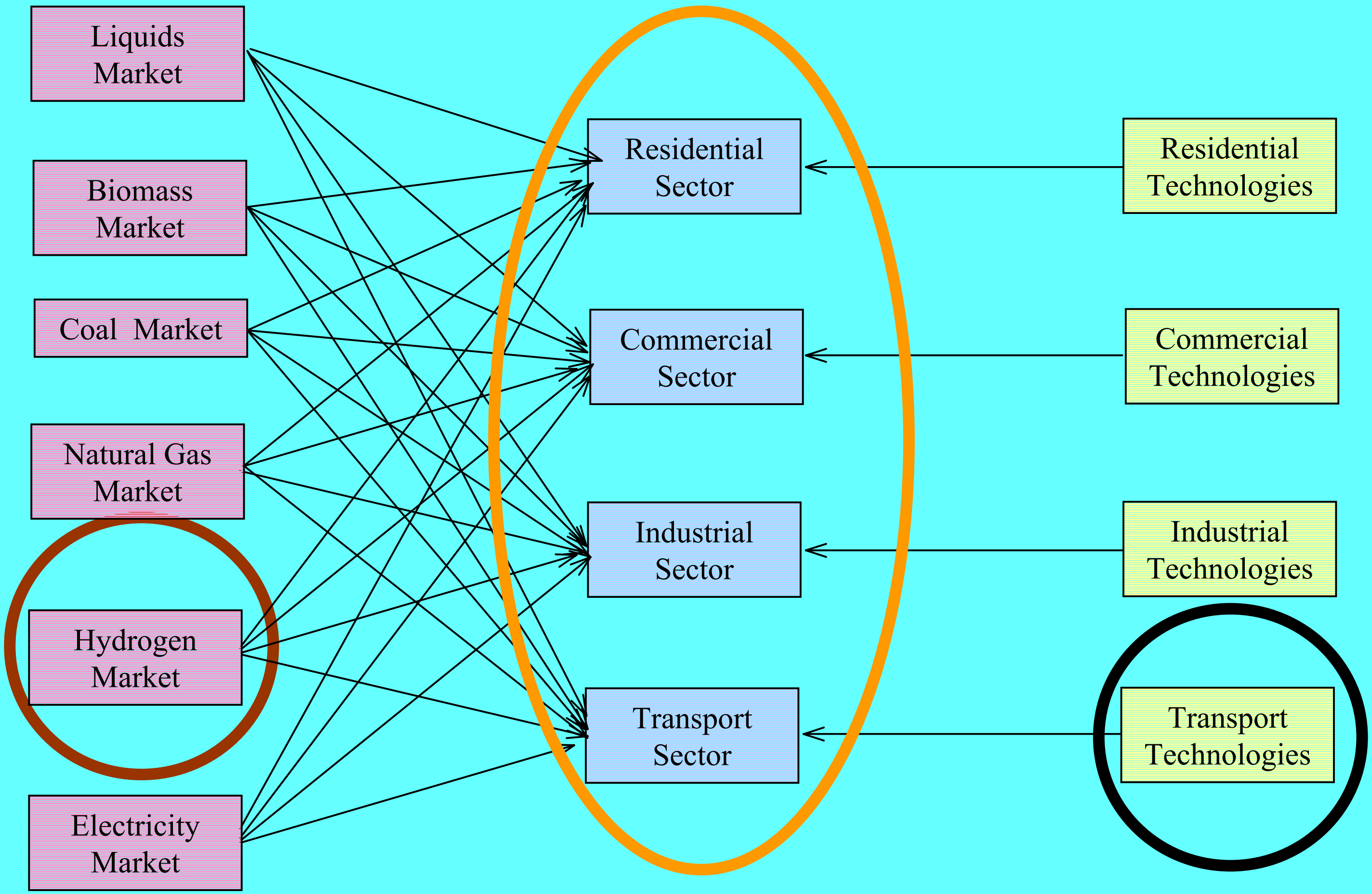
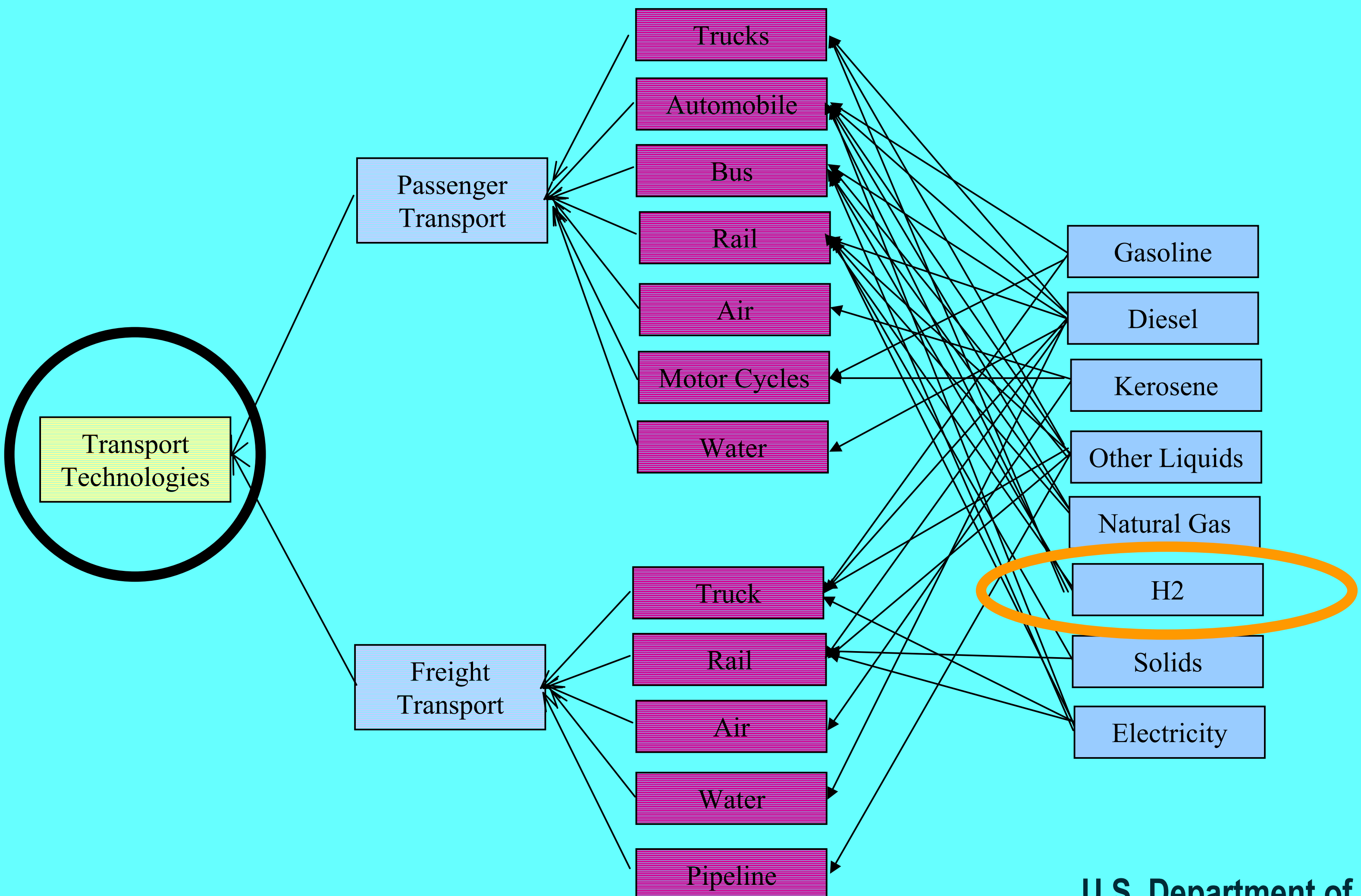
Energy supply pathway options in MiniCAM



Transportation sector detail in MiniCAM



The National Academy of Engineering Study

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Advisers to the Nation on Science, Engineering, and Medicine

February 2004

The Hydrogen Economy: Opportunities, Costs, Barriers, and R&D Needs--*Summary*

BOARD ON ENERGY AND ENVIRONMENTAL SYSTEMS

- Focus on transportation
- Two primary pathways
  - Central H_2 production with pipeline distribution
    - –Natural Gas (with or without CO_2 Capture & Storage)
    - –Coal (with or without CO_2 Capture & Storage
    - –Nuclear (Wind and Solar also included in MiniCAM)
  - Distributed H_2 production with on site production
    - –Electrolysis
    - –Natural Gas (CO_2 emissions)
- Detailed estimates of technology options and associated costs

From the NAE Study to ObjECTS.MiniCAM

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Modeling Insights from ObjECTS.MiniCAM (Preliminary)

- The introduction of NAE optimistic cost estimates into **ObjECTS.MiniCAM** was consistent with **rapid penetration of H_2 into both stationary and mobile transport markets after 2015** (when the NAE assumed these technologies might become available).
  - Total global market H_2 consumption in 2035 exceeds 10 EJ/year.
  - Half of global automobile transportation by 2050 was provided by H_2.
- Given the NAE cost estimates both central station and distributed H_2 production coexist in **ObjECTS.MiniCAM** runs.
- But, central station earns the larger market share in **ObjECTS.MiniCAM** under NAE cost and performance assumptions, due at least in part to its advantages in stationary fuel cell applications.
- The development of a H_2 economy in **ObjECTS.MiniCAM** has:
  - A depressing effect on oil demand.
  - Modest effect on global CO_2 emissions (20% reductions) absent policy.
- Climate policy has only a modest influence on market penetration.

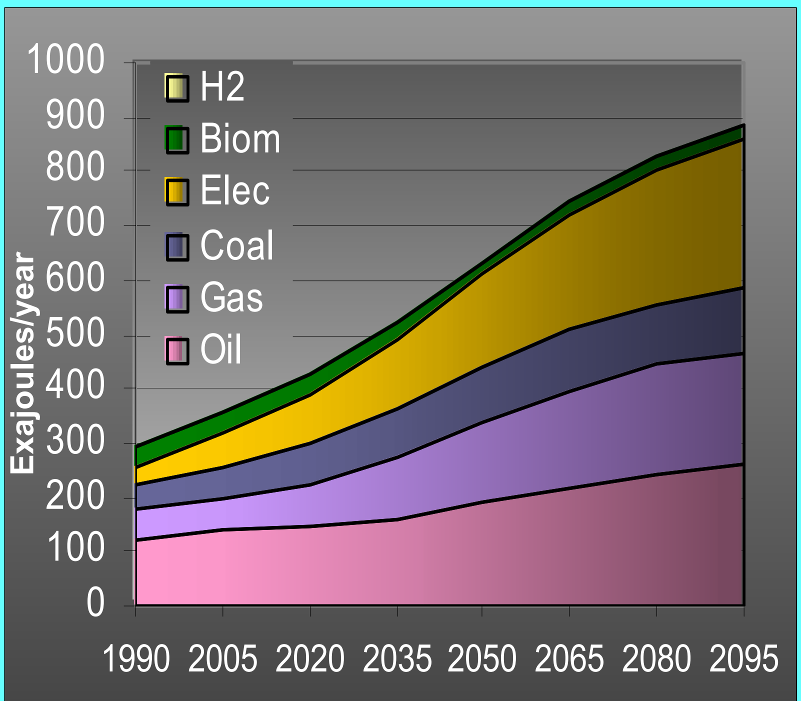
Additional Insights (Preliminary)

- Climate policy will not create a hydrogen economy, the technology must be able to compete in a non-climate constrained world.
- Even if technical hurdles are overcome and hydrogen technology is competitive, a hydrogen economy may not reduce net carbon emissions without a carbon constraint.
- The addition of a climate constraint may actually reduce hydrogen production.
- Hydrocarbon feedstocks (natural gas, coal, and biomass) look particularly attractive as a source of hydrogen.
- Initial deployments may occur in stationary applications.
- Massive deployment in the transportation sector will take time.

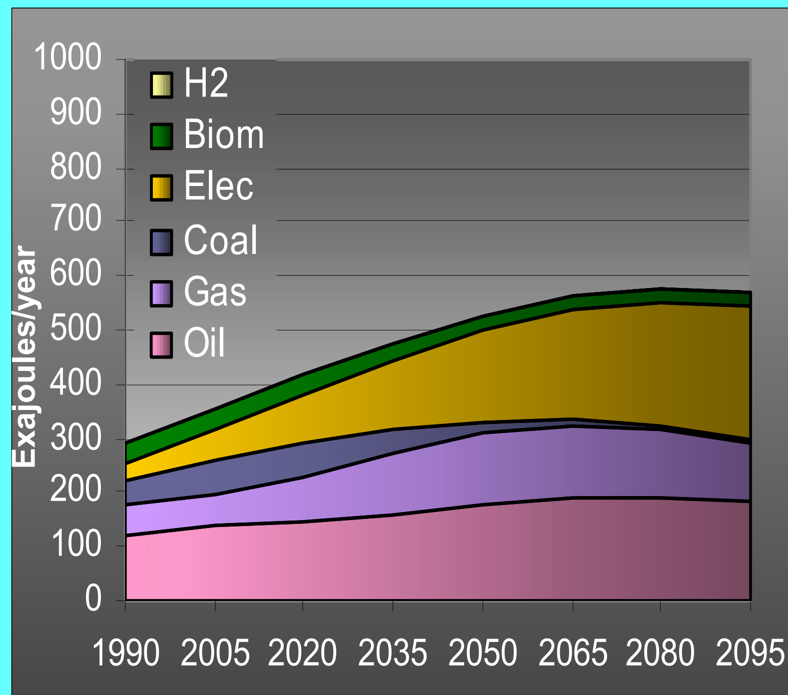
Initial Findings

Climate change policy alone does not necessarily create a market for hydrogen—the technology has to be market competitive without climate policy.

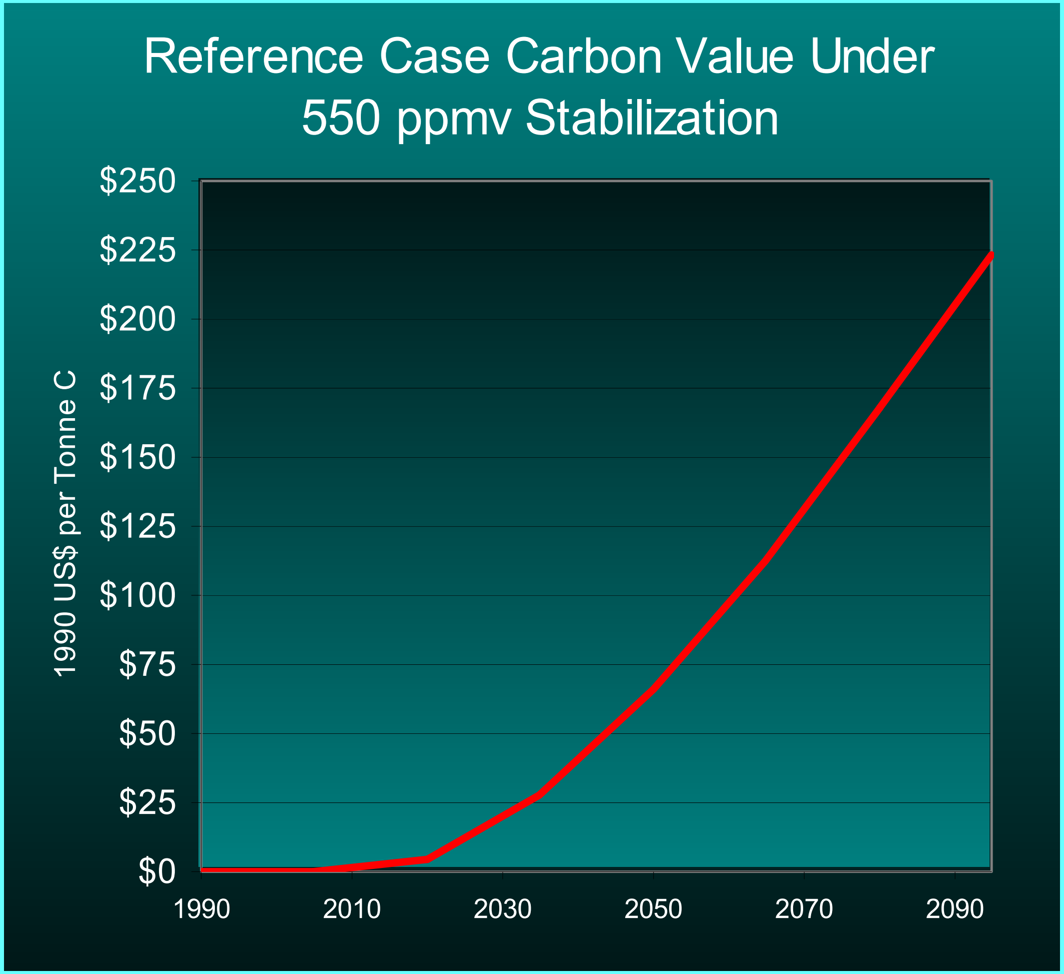
Reference Case, End-use Energy



Reference Case Technology, End-use Energy—550 ppm CO_2



Initial Findings

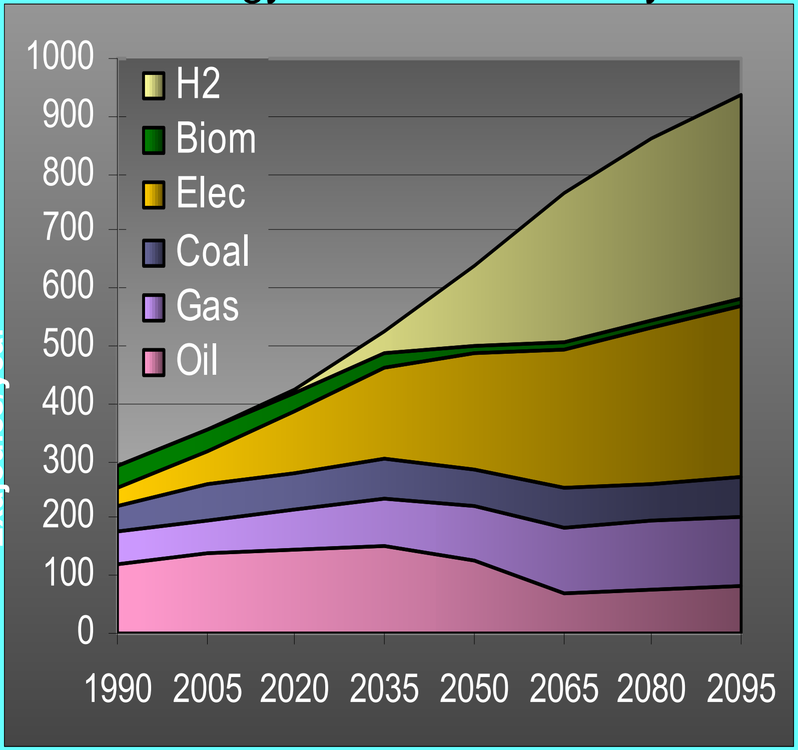


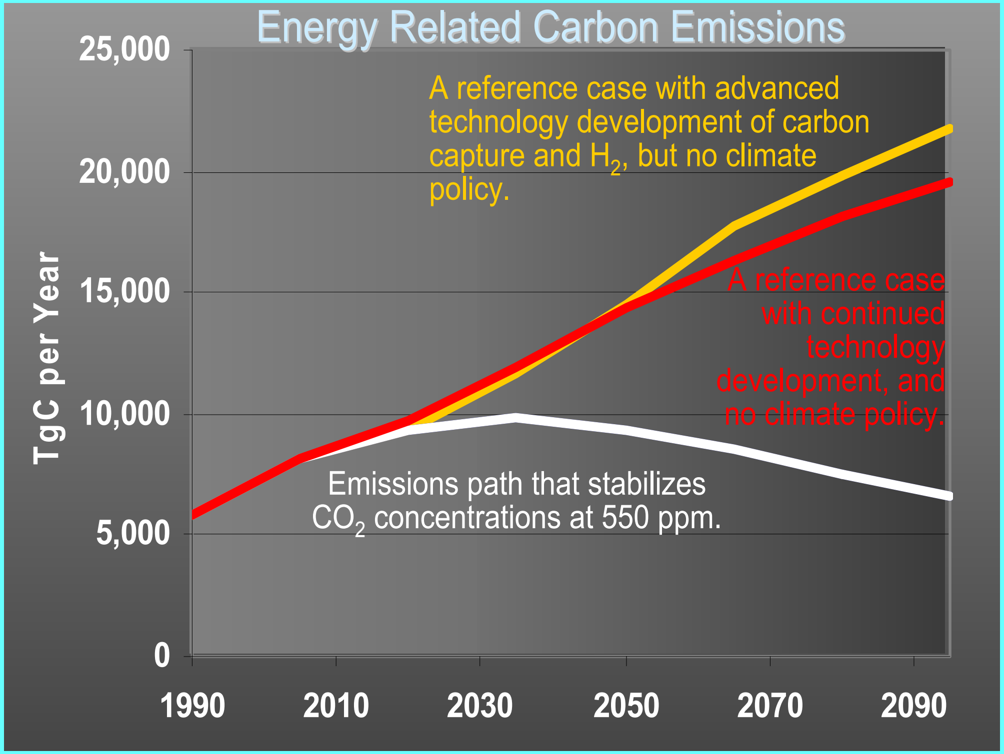
- The carbon value penalizes hydrogen too!
- Where did the H_2 come from?
  - Hydrocarbons (natural gas and coal), or
  - Electricity (which in turn came from power production using fossil fuels).

Initial Findings

The emergence of a hydrogen economy does not necessarily imply reductions in carbon emissions.

H_2 and CCS Technology Case, End-use Energy—No Climate Policy





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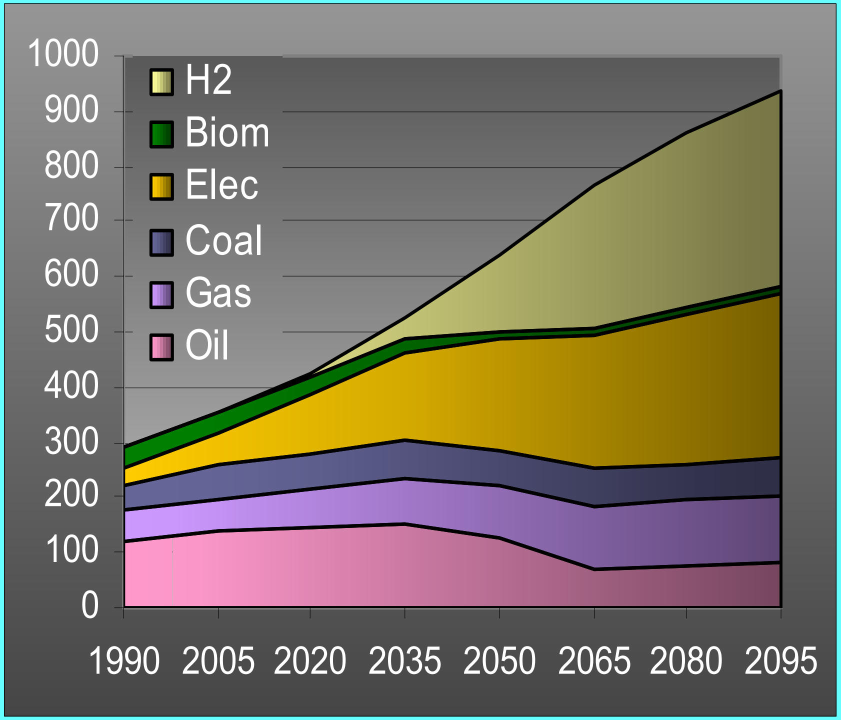
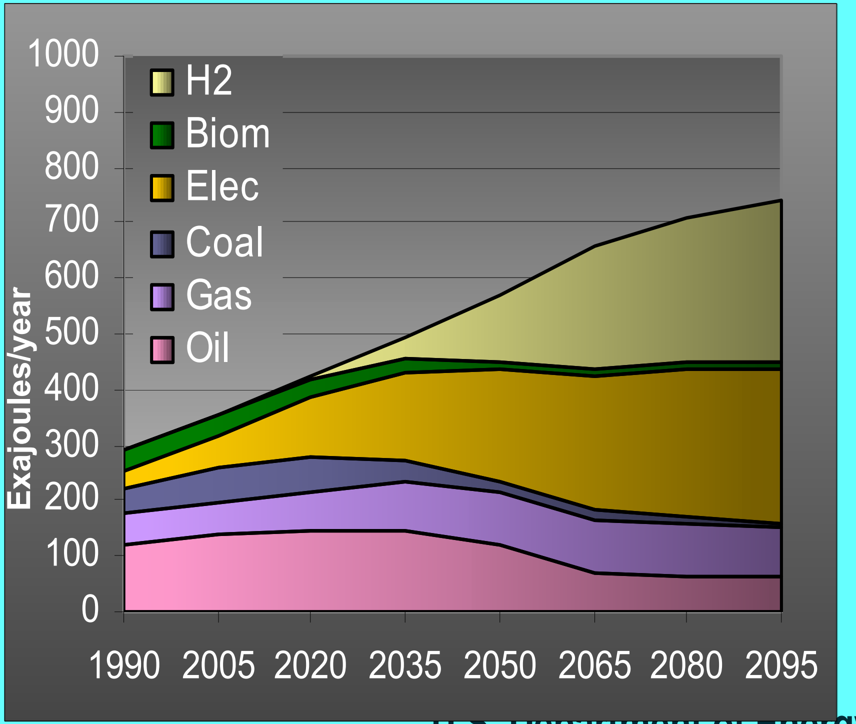
The introduction of a carbon constraint may actually reduce the deployment of hydrogen, although H_2 maintains relative market share

H_2 and CCS Technology Case, End-use Energy—No Climate Policy



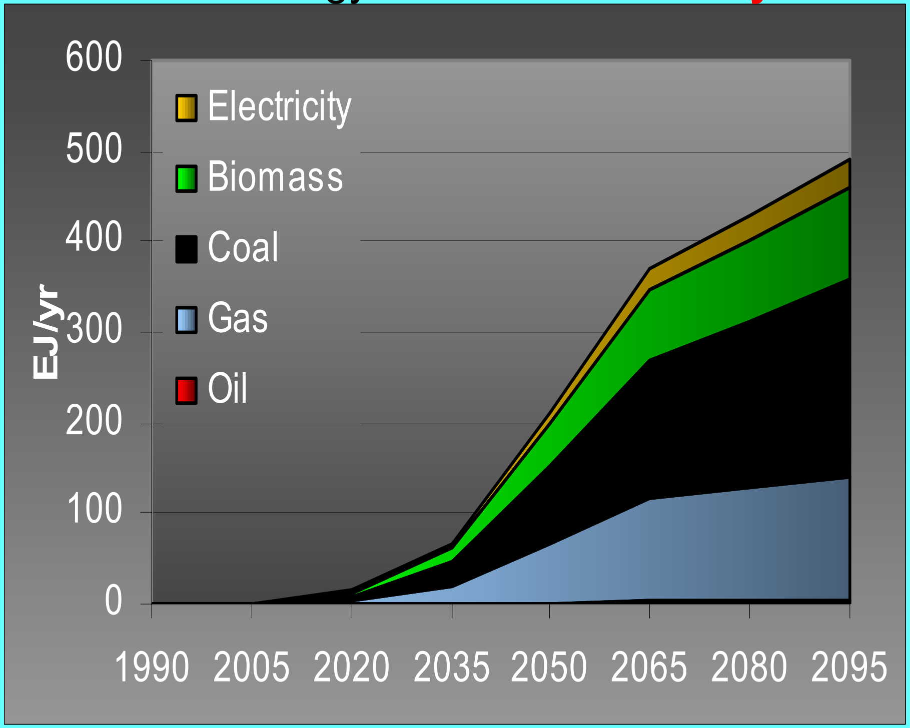
H_2 & CCS Technology Case End-use Energy—550 ppm CO_2



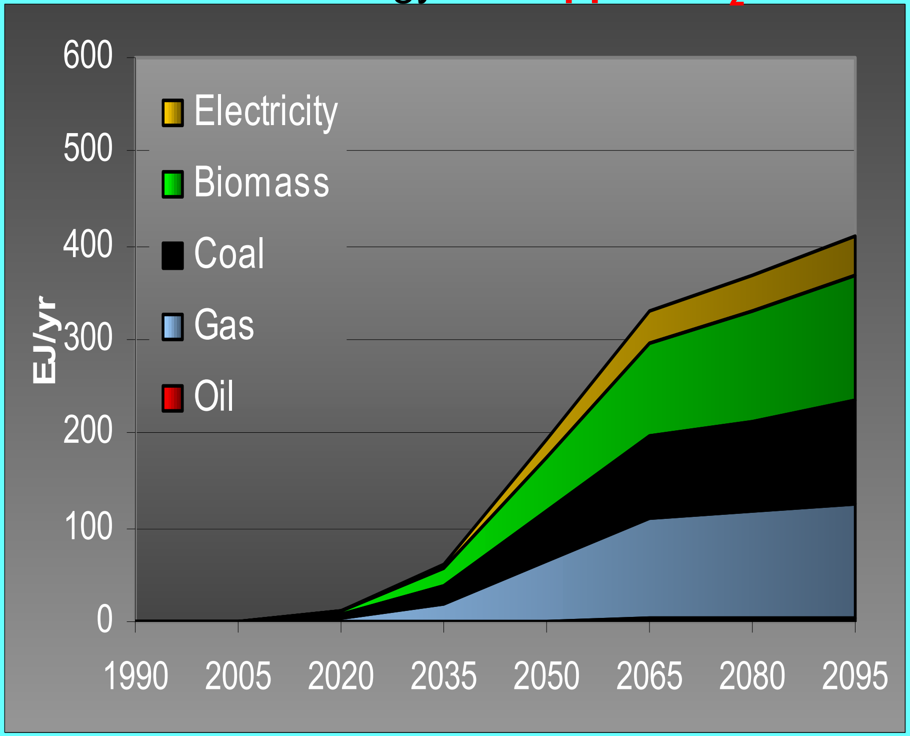
Initial Findings

Hydrocarbons may be the most attractive hydrogen feedstocks. The composition shifts toward bio-fuels in a climate-constrained world.

H_2 and CCS Technology Case, End-use Energy—**No Climate Policy**



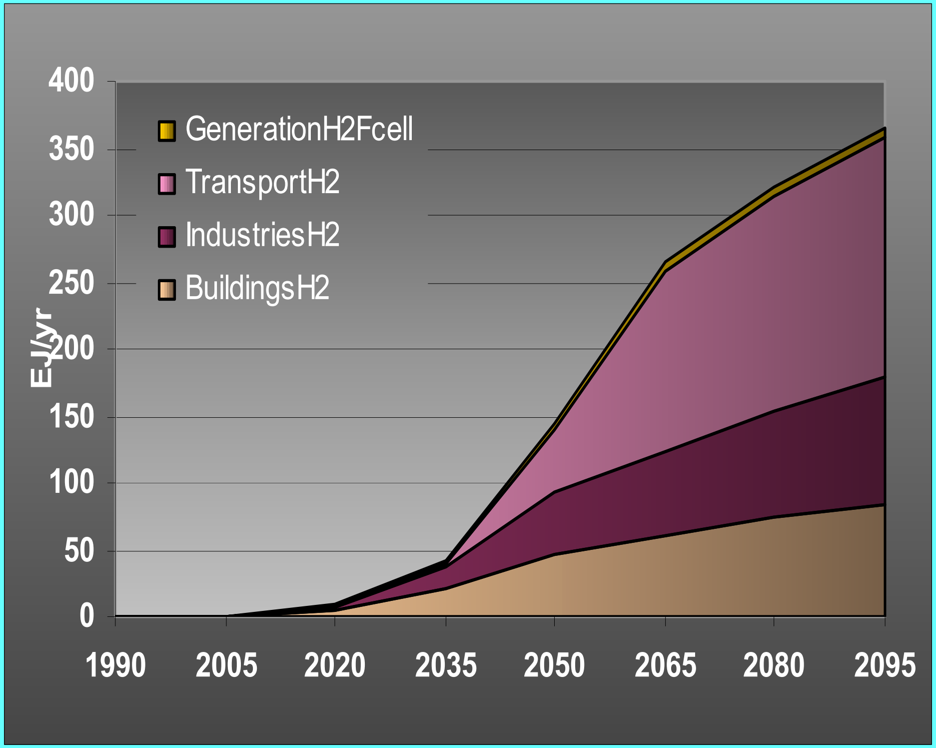
H_2 & CCS Technology Case End-use Energy—**550 ppm CO_2**



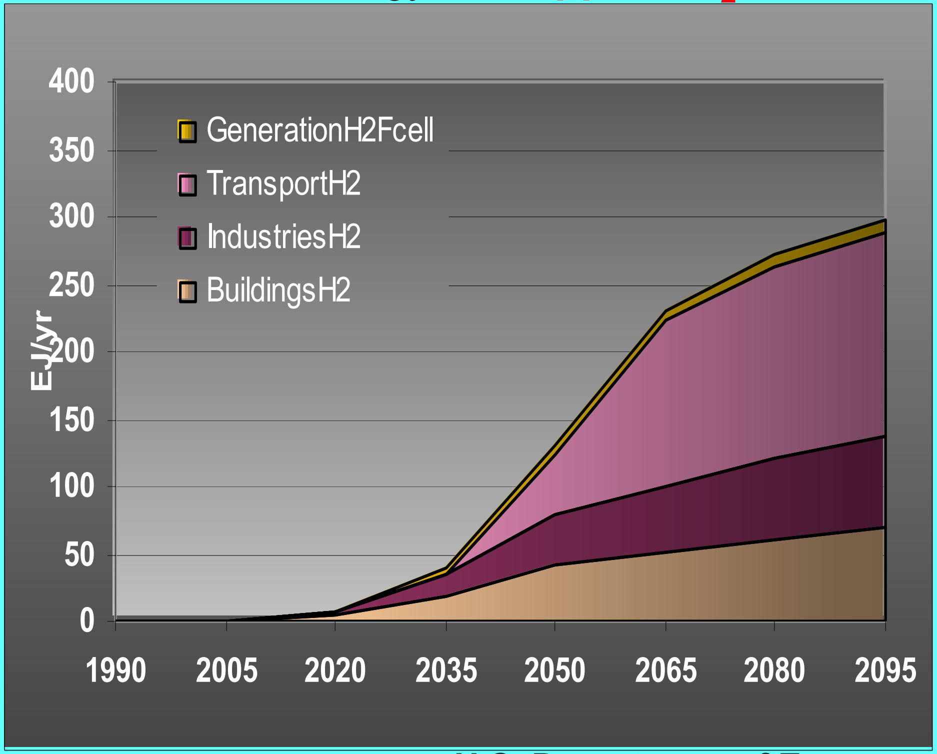
Initial Findings

Significant deployment of hydrogen in transportation systems will take time with or without climate policy.

H_2 and CCS Technology Case, End-use Energy—**No Climate Policy**



H_2 & CCS Technology Case End-use Energy—**550 ppm CO_2**



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- Additional information on the GTSP and a listing of sponsors and collaborators can be found at www.battelle.org/gtsp

Past Systems Analysis Studies

PNNL analysis strengths are based on a history of application to complex energy challenges

- Advanced systems and emerging technologies, where data and experience is less well developed
- New system configurations or applications that must interface with existing subsystems and/or infrastructure
- Requirements to understand and evaluate energy, environmental and economic impacts – in a way that allows effective comparison among technology options
- From design to development to deployment – the need to identify and address institutional and socioeconomic challenges

Technology Characterizations and Market Assessments

Selected examples:

- Life-Cycle Cost Comparisons of Advanced Storage Batteries and Fuel Cells for Utility, Stand-Alone, and Electric Vehicle Applications *(Client: US DOE)*
- Fuel Cells: Performance and Market Assessment *(Client: Portland General Electric)*
- Review of Methods for Forecasting the Market Penetration of New Technologies (*Client: US DOE)*
- Identification and Evaluation of Technologies for CO_2 Control at Fossil-Fuel Power Plants *(Client: Tokyo Electric Power)*
- Site-Specific Economic Assessment of Distributed Generation Technologies *(Client: Toyota Motor Sales, USA)*
- Competitive Intelligence of Battelle's MicroTechnology: Transportable Energy Applications of Proton Exchange Membrane (PEM) Fuel Cells *(Internal PNNL study)*

Energy Systems Analysis

Selected examples:

- Total Energy Cycle Assessment of Electric and Conventional Vehicles: An Energy and Environmental Analysis (with NREL, ANL)
- Lifecycle Assessment of Building Technologies
- Fuel Cycle Evaluations of Biomass-Ethanol and Reformulated Gasoline (with NREL, ORNL)
- Life-cycle Assessment of 1,4-Butanediol Produced from Petroleum Feedstocks Versus Bio-Derived Feedstocks
- Cost and Energy Consumption Estimates for the Aluminum-Air Battery Anode Fuel Cycle